Sensitivity Analysis in Modeling the Fate and Transport of Chemical and Biological Agents

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We are focusing on a problem of importance to national security: the dispersion of chemical or biological agents in the atmosphere, in conjunction with the large, sophisticated computational models used by NARAC. The project is intended as a logical first step for exploring the reduction-to-practice of sensitivity theory to national/homeland security applications.

In the first year, we focused on investigating the use of first-order sensitivity analysis to examine the effect of small perturbations in input parameters on the output of the problem. In the second year we shifted the focus to sensitivity and uncertainty analysis of multidimensional, multivariate, time-dependent wind fields, because these play a dominant role in the uncertainty of atmospheric dispersion prediction. We focused on building a tool from existing methods to characterize and reduce a large multivariate meteorological time series.

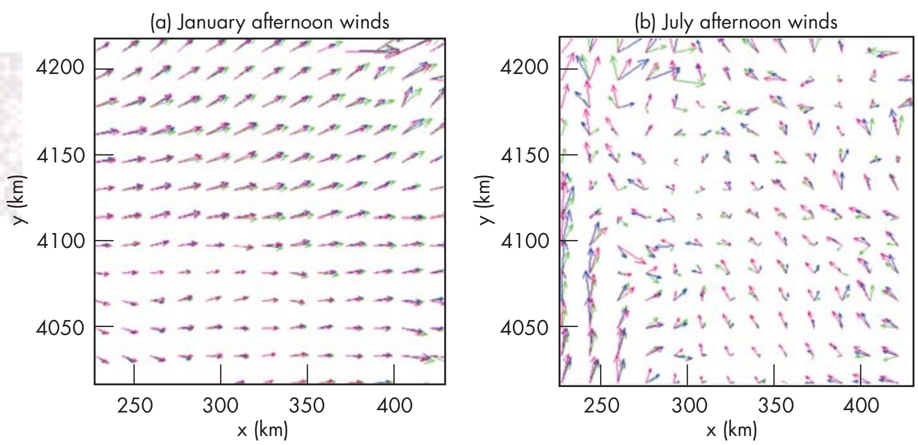

Figure 1. Time-varying wind fields on (a) January and (b) July afternoons at 406-m altitude (3 p. m. in magenta, 4 p. m. in blue, 5 p. m. in green). Domain shown is ~200 km on a side; center magenta wind vector in January is ~5m/s.

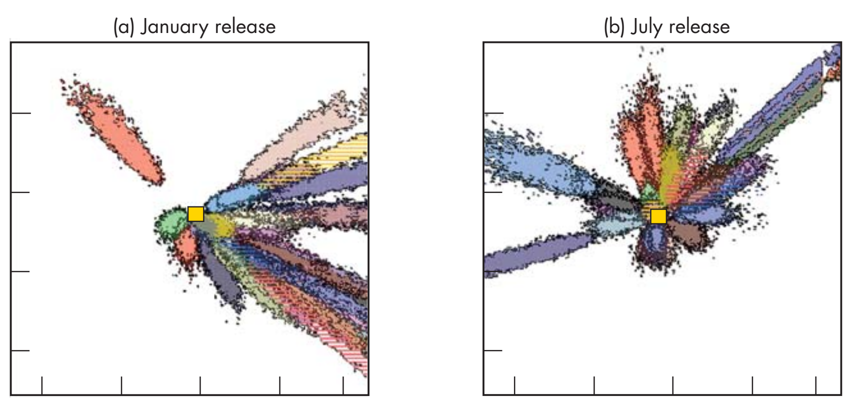

Figure 2. Ensemble of deposition results of 100- to 200-μm particles instantaneously released aloft for 30 days in (a) January and (b) July. Domain shown is 45 km × 45 km. The yellow box marks the release point.

Project Goals

The project goals for FY2004 were: finalization of choice of method to produce representative reduction from large datasets; implementation of statistical tools in stages; testing and analysis to investigate the validity and limitations of the tool; and an exit plan and plan for technology transfer.

Relevance to LLNL Mission

The data reduction tool that we apply for this project will be applicable to other systems both within and outside of LLNL. Efforts from this technology-base project helped to secure funding for a large NAI project beginning in FY2005.

FY2004 Accomplishments and Results

Different methods to classify wind fields over a location include principal component analysis and cluster analysis.

We used an existing extensive wind-field dataset. These wind data vary on both an hourly basis and on a seasonal basis (Fig. 1). While obvious wind patterns can be discerned, a quantitative method for classifying the wind magnitude, direction and duration is desirable.

Cluster analysis divides a set of observations such that most pairs of observations in the same cluster are more similar to each other than are pairs of observations in two different clusters. Prior to clustering, we used Principal Component Analysis (PCA) to reduce the effective dimension of the dataset.

For this study we used a large set of hind-cast wind-field data and an ensemble of dispersion simulations over a specific region over the entire year of 2003. Using a *K*-means method, we partitioned the entire year's worth of noon and midnight data into distinct clusters which are then characterized by probability distributions that describe spatially varying wind speed and direction. The *u*-*v* wind data are plotted in Fig. 3 for the center "release" location of the domain illustrated in Fig. 2.

While clustering was done for the entire year, it is instructive to demonstrate (Fig. 4) how the clustering scheme separates the frequency of wind classes in distal months January and July.

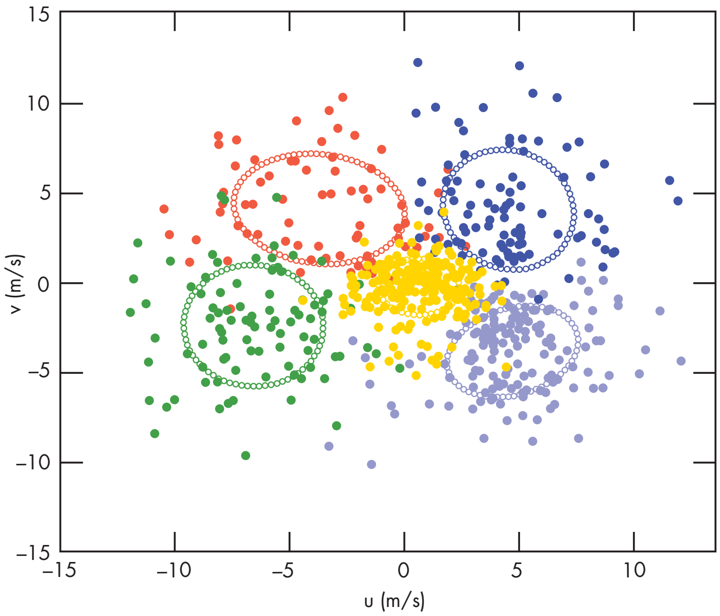

Figure 3. The 2003 *u-v* wind data for 12 p. m. and 12 a. m. wind forecasts at 187-m altitude for the center "release" location. Note 50th percentile contours for the five clusters are indicated by the colored ellipses.

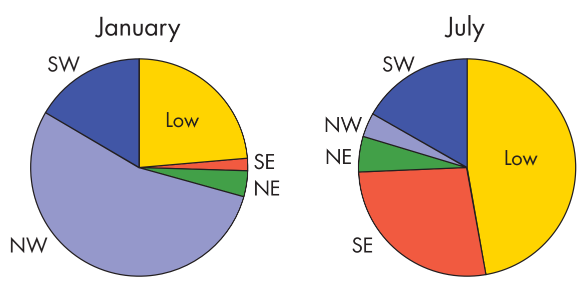

Figure 4. Wind cluster frequency during January and July. January is dominated by westerly winds (70%) and low winds (25%). July is dominated by low winds (50%) and southerly winds (40%). This indicates a lack of synoptic forcing during the summer months and the dominance of local wind patterns in the region. Westerly synoptic forcing dominates during winter months.

The *K*-means clustering method (with and without PCA pretreatment) is effective in using a heterogeneous high-dimensional multivariate data set to create a manageable set of relatively homogeneous classes which can be characterized stochastically and used in event planning and consequence assessments as well as in sensitivity/uncertainty analyses. The method can easily be modified to account for additional altitudes, a vertical velocity component, and shorter time steps.

Related References

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